

Electric Dipolar Susceptibility of the Anderson-Holstein Model

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The temperature dependence of electric dipolar susceptibility χ_P is discussed on the basis of the Anderson-Holstein model with the use of a numerical renormalization group (NRG) technique. Note that χ_P is related with phonon Green's function D . In order to obtain correct temperature dependence of χ_P at low temperatures, we propose a method to evaluate χ_P through the Dyson equation from charge susceptibility χ_c calculated by the NRG, in contrast to the direct NRG calculation of D . We find that the irreducible charge susceptibility estimated from χ_c agree with the perturbation calculation, suggesting that our method works well.

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In the research field of condensed matter physics, exotic magnetism in cage structure materials such as filled skutterudites has attracted much attention due to the interests on new electronic properties caused by oscillation of a guest atom in a cage composed of relatively light atoms [1]. Such oscillation with large amplitude is frequently called *rattling* and it is considered to play crucial roles for the formation of magnetically-robust heavy electron state in $\text{SmOs}_4\text{Sb}_{12}$ [2]. This peculiar heavy-electron state has been theoretically investigated from various aspects by several groups [3–17].

Recently, the Kondo effect of a *vibrating* magnetic ion in a cage has been theoretically discussed on the basis of a two-channel conduction electron system hybridized with a vibrating magnetic ion [18–20]. Note here that a vibrating ion inevitably induces electric dipole moment. Then, it has been found that magnetic and non-magnetic Kondo effects alternatively occur due to the screening of spin moment and electric dipole moment of vibrating ion [21]. In particular, electric dipolar two-channel Kondo effect has been found to occur for weak Coulomb interaction. Then, it has been proposed that magnetically robust heavy-electron state appears near the fixed point of electric dipolar two-channel Kondo effect.

In this paper, in order to promote our understanding on the Kondo effect concerning electric dipole moment P , we analyze the temperature dependence of electric dipolar susceptibility χ_P on the basis of the Anderson-Holstein Hamiltonian with the use of a numerical renormalization group method. For the reproduction of correct temperature dependence of χ_P at low temperatures, we propose a method to evaluate χ_P through the Dyson equation from charge susceptibility χ_c . This method is found to provide correct results in the temperature region lower than the Kondo temperature, in sharp contrast to the numerical evaluation of the phonon Green's function which is directly related to χ_P .

Now we explain the model Hamiltonian. We consider a conduction electron system in which an impurity ion

is embedded. On the impurity site, localized electrons are coupled with ion vibration. The situation is well described by the Anderson-Holstein model, given by [22]

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + V \sum_{\mathbf{k}\sigma} (c_{\mathbf{k}\sigma}^\dagger d_\sigma + \text{h.c.}) + H_{\text{loc}}, \quad (1)$$

where $\varepsilon_{\mathbf{k}}$ is the dispersion of conduction electron, $c_{\mathbf{k}\sigma}$ is an annihilation operator of conduction electron with momentum \mathbf{k} and spin σ , d_σ denotes an annihilation operator of the localized electron with spin σ , and V is the hybridization between conduction and localized electrons. The local term H_{loc} is given by

$$H_{\text{loc}} = \mu\rho + gx\rho + p^2/2 + \omega^2 x^2/2, \quad (2)$$

where μ is a chemical potential, $\rho = \sum_\sigma n_\sigma$ with $n_\sigma = d_\sigma^\dagger d_\sigma$, g denotes the coupling between electron density and ion vibration, x is normal coordinate of the vibrating ion, p indicates the corresponding canonical momentum, and ω is the vibration energy. Note that the reduced mass of the vibrating ion is set as unity.

In the present model, we ignore the Coulomb interaction term $Un_\uparrow n_\downarrow$. Of course, the effect of U is quite important, but our main purpose here is to understand the temperature dependence of electric dipolar susceptibility χ_P . Since χ_P should be affected by U , it is necessary to grasp in the first place the temperature dependence of χ_P without the effect of U . Thus, in the present work, the Coulomb interaction is ignored. The effect of U will be discussed elsewhere in future.

For actual calculations, it is convenient to introduce phonon operator b and b^\dagger through the relation of $x = (b + b^\dagger)/\sqrt{2\omega}$. Then, the local term is rewritten as

$$H_{\text{loc}} = \mu\rho + \sqrt{\alpha}\omega\rho(b + b^\dagger) + \omega(b^\dagger b + 1/2), \quad (3)$$

where α is the non-dimensional electron-phonon coupling, defined by $\alpha = g^2/(2\omega^3)$. Concerning the average electron number, throughout this paper, we consider the half-filling case, at which μ is given by $\mu = 2\alpha\omega$.

The conduction electron model hybridized with local impurity is precisely analyzed with the use of a numerical renormalization group (NRG) technique [23, 24].

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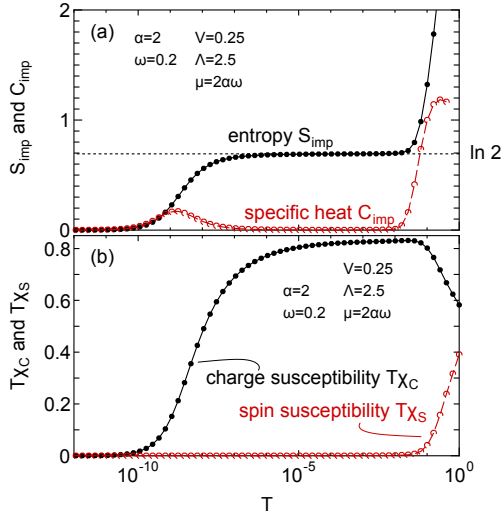


FIG. 1: (Color online) (a) Entropy S_{imp} and specific heat C_{imp} vs. temperature T for $\alpha = 2$ and $\omega = 0.2$. (b) Charge susceptibility $T\chi_c$ and spin susceptibility $T\chi_s$ vs. temperature T for the same parameters as (a).

The logarithmic discretization of the momentum space is characterized by a parameter Λ and we keep M low-energy states for each renormalization step. Throughout this paper, Here we set $\Lambda=2.5$ and $M=5000$. The energy unit is a half-bandwidth of the conduction electron. In this unit, we fix V as $V = 0.25$. As for the calculation of phonon part, the number of basis is 50.

In order to clarify electronic properties of H , first we evaluate entropy S_{imp} and specific heat C_{imp} , which are given by $S_{\text{imp}} = -\partial F / \partial T$ and $C_{\text{imp}} = -T \partial^2 F / \partial T^2$, respectively, where F is the free energy of local electron and T is a temperature, defined by $T = \Lambda^{-(N-1)/2}$ with the renormalization step number N . We also evaluate charge and spin susceptibilities, χ_c and χ_s , which are, respectively, given by

$$\chi_c = \frac{1}{Z} \sum_{ij} \frac{e^{-E_i/T} - e^{-E_j/T}}{E_j - E_i} |\langle i | \rho - \langle \rho \rangle | j \rangle|^2, \quad (4)$$

and

$$\chi_s = \frac{1}{Z} \sum_{ij} \frac{e^{-E_i/T} - e^{-E_j/T}}{E_j - E_i} |\langle i | s_z | j \rangle|^2, \quad (5)$$

where E_i is the eigen-energy of H , $|i\rangle$ is the corresponding eigen-state, Z is the partition function given by $Z = \sum_i e^{-E_i/T}$, $\langle \rho \rangle = \sum_i \langle i | \rho | i \rangle e^{-E_i/T} / Z$, and $s_z = n_\uparrow - n_\downarrow$.

Now we move on to the NRG results. First we show typical results for the Kondo phenomenon due to the electron-phonon coupling. In Fig. 1(a), we depict S_{imp} and C_{imp} as functions of T for $\alpha = 2$ and $\omega = 0.2$. In the high- T region as $T \gtrsim 10^{-2}$, S_{imp} shows a large value due to phonon excited states. For $10^{-7} \lesssim T \lesssim 10^{-2}$, S_{imp} indicates a plateau of $\ln 2$ and C_{imp} becomes almost zero in the corresponding temperature region. Note that

we do not understand what degree of freedom is relevant to $\ln 2$ only from the results of S_{imp} and C_{imp} . This point will be discussed later. Around at $T = 1.8 \times 10^{-9}$, we observe the release of entropy $\ln 2$ and the specific heat C_{imp} forms a clear peak, which defines the Kondo temperature T_K . Thus, we obtain $T_K = 1.8 \times 10^{-9}$ for the present parameters. Finally, for $T \lesssim 10^{-9}$, both S_{imp} and C_{imp} vanish, indicating that the system is in the local Fermi-liquid state.

In order to clarify the degree of freedom relevant to the present Kondo phenomenon, we evaluate charge and spin susceptibilities. The results are shown in Fig. 1(b). We immediately notice that the spin susceptibility χ_s is rapidly suppressed even at high temperatures as $T \sim 10^{-1}$, when we decrease the temperature. On the other hand, the charge susceptibility χ_c is rather increased to the enhanced value for $T \sim 10^{-2}$. In the temperature range of $10^{-7} \lesssim T \lesssim 10^{-2}$ in which $\ln 2$ plateau appears, we find the large value of χ_c . Around at $T = T_K$, we observe that χ_c is gradually suppressed. Namely, the Kondo behavior clearly appears in the temperature dependence of χ_c . We conclude that in the present model, the charge Kondo effect occurs, since degenerate vacant and double occupied states play roles of pseudo spins.

As for the understanding of the charge Kondo effect, it seems to be enough to evaluate χ_c . However, in order to visualize the situation of the charge Kondo effect, it is useful to recall that the vibrating ion induces electric dipole moment P , given by $P = zex$, where z denotes the valence of the guest ion, e indicates electron charge, and x is ion displacement. Namely, the electric dipole susceptibility χ_P is also related to the Kondo effect for the vibrating ion problem [21]. As easily understood from the definition of P , we obtain χ_P as

$$\chi_P = \frac{(ze)^2}{2\omega} D, \quad (6)$$

where D denotes the zero-energy component of the phonon Green's function, given by

$$D_{\text{NRG}} = \frac{1}{Z} \sum_{ij} \frac{e^{-E_i/T} - e^{-E_j/T}}{E_j - E_i} |\langle i | u - \langle u \rangle | j \rangle|^2. \quad (7)$$

Here u is given by $u = b + b^\dagger$ and we add a subscription "NRG" to show explicitly that this quantity is evaluated by the NRG method.

Of course, we can perform the NRG calculation for D_{NRG} , but we consider an alternative way to evaluate χ_P without using D_{NRG} . For the purpose, we exploit the Dyson equation, which relates χ_c and D . In general, the Dyson equations are diagrammatically shown in Fig. 2 and the first one (a) is expressed by

$$D(i\nu_n) = D_0(i\nu_n) + g^2 D_0(i\nu_n)^2 \Pi(i\nu_n), \quad (8)$$

where $\nu_n = 2\pi T n$ is the boson Matsubara frequency with an integer n , D is the dressed phonon Green's function, g is the electron-phonon coupling constant, Π denotes

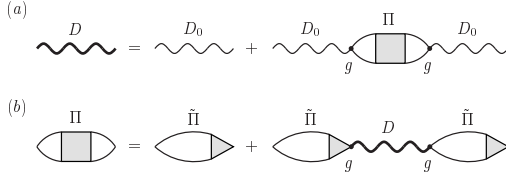


FIG. 2: Dyson equations for phonon Green's function D (thick wavy line) and polarization function Π (bubble with hatched square). Thin wavy line and bubble with hatched triangle denote non-interacting phonon Green's function D_0 and irreducible polarization function $\tilde{\Pi}$, respectively.

polarization function, and D_0 is a non-interacting phonon Green's function, given by $D_0(i\nu_n) = -2\omega/[(i\nu_n)^2 - \omega^2]$. At the static limit of $\nu_n = 0$, by noting that $\Pi(0) = \chi_c$, $D_0(0) = 2/\omega$, and $g = \sqrt{\alpha}\omega$, we obtain a relation between D and χ_c as

$$D = 2/\omega + 2\alpha\chi_c. \quad (9)$$

In principle, D of eq. (9) is equal to D_{NRG} of eq. (7).

In Fig. 3, we depict TD_{NRG} and TD vs. T for $\omega = 0.2$ for the comparison of D_{NRG} and D . We show a couple of results for $\alpha = 1$ and 2. In the high- T region, we find that TD_{NRG} and TD agree well with each other. To be honest, we observe a little quantitative difference between TD_{NRG} and TD , although it is difficult to notice it in the graph of the logarithmic scale. This type of small deviation can be overcome by the elevation of the numerical accuracy. For instance, if we keep more numbers of states in each renormalization step, the accuracy is expected to be improved.

However, in the low-temperature region of $T < T_K$, where $T_K = 1.8 \times 10^{-9}$ for $\alpha = 2$ and $T_K = 6.6 \times 10^{-4}$ for $\alpha = 1$, we observe serious discrepancy between TD_{NRG} and TD . From the analysis of numerical data, we find that $TD_{\text{NRG}} \propto T^2$ and $TD \propto T$ for $T < T_K$. When we fix a temperature and increase α , both TD_{NRG} and TD are monotonic increasing functions. The slope of TD_{NRG} or TD seems to be independent to α .

This difference seems to be so serious that it is difficult to determine which is the correct behavior. However, here we recall the local Fermi-liquid theory for $T < T_K$. Namely, we obtain the narrow quasi-particle band at the Fermi level in the electron density of states, leading to constant density of states ρ_0 . Since χ_c can be related to ρ_0 at low temperatures, it is natural to consider that D should be constant at the same temperature region. If we further imagine that phonon frequency $\tilde{\omega}$ is decreased due to the Kondo screening, the dressed phonon Green's function $D = 2/\tilde{\omega}$ should be larger than $D_0(0) = 2/\omega$. We deduce that $\tilde{\omega}/\omega$ is a monotonic decreasing function of α . In short, it seems to be natural to consider that $TD \propto T$ in the charge Kondo effect.

If so, here we have a naive question concerning the reason why we cannot evaluate correctly D by the NRG method. In eq. (7), D_{NRG} can be calculated in the NRG

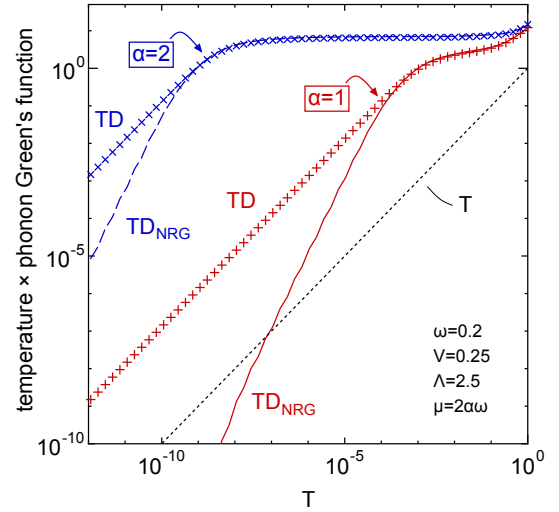


FIG. 3: (Color online) D and D_{NRG} vs. temperature T for $\omega = 0.2$. The solid (dashed) curve indicates TD_{NRG} for $\alpha = 1$ (2), while the cross (plus) indicates TD for $\alpha = 1$ (2).

method, but it includes implicit problems in the calculation accuracy. In the NRG method, in order to deal with the states which increase rapidly in each renormalization step, only M low-energy states are kept and the rests are simply discarded. In the renormalization process, the electron-phonon excited states which are indispensable for the description of phonon excitation will be lost. This type of problem has been already pointed out in the analysis of the two-channel model [21]. On the other hand, since the local charge susceptibility χ_c is the physical quantity with large contribution from the electron states near the Fermi level, we expect that χ_c is obtained in good accuracy with the use of NRG method.

Let us check the NRG calculation from a different viewpoint by the comparison with the perturbation calculation. Here we define the irreducible polarization function $\tilde{\Pi}(i\nu_n)$, which is related with Π and D through the Dyson equation (b) in Fig. 2 as

$$\Pi(i\nu_n) = \tilde{\Pi}(i\nu_n) + g^2 \tilde{\Pi}(i\nu_n)^2 D(i\nu_n). \quad (10)$$

At $\nu_n = 0$, by noting eq. (9) and $\chi_c = \Pi(0)$, we obtain

$$\tilde{\chi}_c^{-1} = \chi_c^{-1} + 2\alpha\omega, \quad (11)$$

where irreducible charge susceptibility is defined as $\tilde{\chi}_c = \tilde{\Pi}(0)$.

In Fig. 4, we show $\tilde{\chi}_c$ vs. α obtained from eq. (11) with the use of the NRG result of χ_c for $\omega = 0.2$. Note that χ_c at low enough temperature is estimated at $T = 1.1 \times 10^{-10}$. For each value of α , we have checked that $\tilde{\chi}_c$ is unchanged even at lower T . For small α , it is shown that the NRG results agree quite well with the perturbation result in the order of α . For large α , D is enhanced and χ_c becomes large, indicating that $\tilde{\chi}_c$ approaches the value of $1/U_{\text{ph}}$, where U_{ph} denotes the magnitude of attractive interaction, given by $U_{\text{ph}} = 2\alpha\omega$ in the present case. The

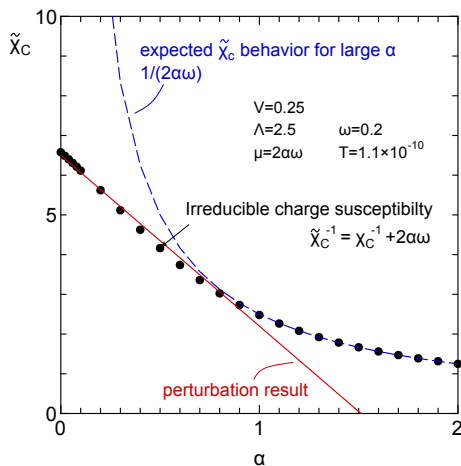


FIG. 4: (Color online) Irreducible charge susceptibility $\tilde{\chi}_c$ (solid circles) vs. α for $T = 1.1 \times 10^{-10}$ and $\omega = 0.2$. The solid line indicates the perturbation calculation result of $\tilde{\chi}_c$ up to the first order of α and the dashed curve means the expected behavior of $\tilde{\chi}_c \sim 1/(2\alpha\omega)$ for large α , respectively.

NRG results for $\tilde{\chi}_c$ reproduce the behavior of $1/U_{\text{ph}}$ for large α . Thus, it is confirmed that χ_c is constant at low temperature from eq. (11).

Finally, let us provide a comment on the effect of Coulomb interaction, which has been completely ignored in this paper. When we include U , we imagine that U_{ph} is

suppressed as $U_{\text{ph}} = 2\alpha\omega - U$. For $U > 2\alpha\omega$, the charge Kondo effect disappears and the spin Kondo effect occurs instead [14]. We think that it is interesting to consider the behavior of χ_P for $U \geq 2\alpha\omega$.

In summary, we have discussed the temperature dependence of electric dipolar susceptibility χ_P of the Anderson-Holstein model with the use of the NRG technique. We consider a direct method to evaluate phonon Green's function D_{NRG} and another indirect way to calculate D from χ_c through the Dyson equation. After careful investigations, we have concluded that D provides correct temperature dependence in contrast to D_{NRG} for T smaller than the Kondo temperature. The effect of the Coulomb interaction on χ_P is one of future problems.

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- [1] See, for instance, *Proceedings of International Conference on New Quantum Phenomena in Skutterudite and Related Systems* (Skutterudite 2007), J. Phys. Soc. Jpn. **77** (2008) Suppl. A.
 - [2] S. Sanada, Y. Aoki, H. Aoki, A. Tsuchiya, D. Kikuchi, H. Sugawara, and H. Sato, J. Phys. Soc. Jpn. **74**, 246 (2005).
 - [3] S. Yotsuhashi, M. Kojima, H. Kusunose, and K. Miyake, J. Phys. Soc. Jpn. **74**, 49 (2005).
 - [4] K. Hattori, Y. Hirayama, and K. Miyake, J. Phys. Soc. Jpn. **74**, 3306 (2005).
 - [5] K. Hattori, Y. Hirayama and K. Miyake, J. Phys. Soc. Jpn. **75** Suppl., 238 (2006).
 - [6] K. Mitsumoto and Y. Ōno, Physica C **426-431**, 330 (2005).
 - [7] K. Mitsumoto and Y. Ōno, Physica B **378-380**, 265 (2006).
 - [8] K. Mitsumoto and Y. Ōno, J. Phys. Soc. Jpn **79**, 054707 (2010).
 - [9] T. Fuse and Y. Ōno, J. Phys. Soc. Jpn. **79**, 093702 (2010).
 - [10] T. Fuse and Y. Ōno, J. Phys. Soc. Jpn. **80**, SA136 (2011).
 - [11] T. Fuse, Y. Ōno, and T. Hotta, J. Phys. Soc. Jpn. **81**, 044701 (2012).
 - [12] T. Hotta, Phys. Rev. Lett. **96**, 197201 (2006).
 - [13] T. Hotta, J. Phys. Soc. Jpn. **76**, 023705 (2007).
 - [14] T. Hotta, J. Phys. Soc. Jpn. **76**, 084702 (2007).
 - [15] T. Hotta, Physica B **403**, 1371 (2008).
 - [16] T. Hotta, J. Phys. Soc. Jpn. **77**, 103711 (2008).
 - [17] T. Hotta, J. Phys. Soc. Jpn. **78**, 073707 (2009).
 - [18] S. Yashiki, S. Kirino, and K. Ueda, J. Phys. Soc. Jpn. **79**, 093707 (2010).
 - [19] S. Yashiki, S. Kirino, K. Hattori, and K. Ueda, J. Phys. Soc. Jpn. **80**, 064701 (2011).
 - [20] S. Yashiki and K. Ueda, J. Phys. Soc. Jpn. **80**, 084717 (2011).
 - [21] T. Hotta and K. Ueda, to appear in Phys. Rev. Lett. (arXiv:1203.4692)
 - [22] We use such units as $\hbar = k_B = 1$.
 - [23] K. G. Wilson, Rev. Mod. Phys. **47**, 773-840 (1975).
 - [24] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980).